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by William F. Ford

Lewis Research Center
Cleveland, Ohio

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by William F. Ford

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio

ABSTRACT

In the complex energy plane, the pure Coulomb T matrix possesses branch points which would not appear if the force were properly defined. This is demonstrated by a study of the screened Coulomb T matrix in the limit as the screening radius R tends to infinity. No branch points develop if the proper order of limiting processes is observed and the results agree with previous calculations; however, the T matrix is discontinuous in the limit. A formula for the screened Coulomb T matrix is given which is valid to order 1/R for all energies.

I. INTRODUCTION

The T matrix for a system undergoing scattering is given by

$$T = V + V \frac{1}{E + i\varepsilon - K - V} V. \tag{1}$$

Here K is the Hamiltonian for the system in the absence of interaction, and V is the interaction giving rise to the scattering. The total energy of the system is denoted by E; the small imaginary term $i\varepsilon$ serves to make the Green's function

$$G = \frac{1}{E + i\varepsilon - K - V} \tag{2}$$

well defined.

We shall consider the T matrix in the momentum representation, with matrix elements denoted by $\langle \underset{\sim}{k}_2 | T | \underset{\sim}{k}_1 \rangle$. It is convenient to introduce a complex wave number k, which is related to the total energy by

$$E + i\varepsilon = \frac{\hbar^2 k^2}{2m}, \qquad 0 < \arg(k) < \pi ;$$

thus the energy dependence of the T matrix may be indicated explicitly by $\langle \underset{\sim}{k}_2 | T(k) | \underset{\sim}{k}_1 \rangle$, or simply T(k).

For most quantum mechanical systems, the T matrix cannot be given in closed form. However, the case of a two-particle system with pure Coulomb interaction has been studied extensively, and recently Hostler and others[1] derived integral representations for the Coulomb Green's function which reduce to hypergeometric functions. From these the Coulomb T matrix can be obtained directly.

The resulting expression for T(k), however, has the drawback that it does not approach a well-defined limit as $k^2 \to k_1^2$ or $k^2 \to k_2^2$, and indeed has branch points there. This behavior is certainly not correct, for one can show on very general grounds that the only singularities of T(k) should be a branch point at $k = 0$ and simple poles on the imaginary k-axis corresponding to the bound state energies of K + V.

The correct form of the T matrix when $k^2 = k_1^2$ is given in Ref. 2, where a similar anomaly in the limiting process $|\underset{\sim}{k}_2| \to |\underset{\sim}{k}_1|$ was studied. The difficulty there was traced back to the long-range nature of the Coulomb force and disappeared when the effects of shielding were introduced.

In the present case the unphysical branch points are also due to neglect of shielding effects. The scattering of charged particles is caused by an interaction which is always screened at very large distances; the T matrix may therefore properly be regarded as depending on two parameters, ϵ and the screening radius R. To find the value of T(k,R) for real k, one must take $\epsilon \to 0$ followed by $R \to \infty$. Usually, the ordering is unimportant, but the branch points at k_1^2 and k_2^2 occur in Hostler's expression because the limit $R \to \infty$ has been (implicitly) taken first.

The present work is intended to clarify the situation by studying the behavior of the screened Coulomb T matrix in the limit $R \to \infty$. In Sec. II the formalism is established and applied to the cutoff Coulomb potential. This interaction is chosen because it allows one to determine unambiguously the effects caused by extending the potential past the cutoff radius. In Sec. III these effects are isolated, and a general expression for the screened Coulomb T matrix is derived, which is valid to order 1/R for all k.

In Sec. IV the limits $\epsilon \to 0$ and $R \to \infty$ are taken. We find that branch points at k_1^2 and k_2^2 do not appear if the proper order of limits is used; furthermore, the resulting T matrix agrees with that obtained in Ref. 2. For other values of k, the screened and pure Coulomb T matrices are identical in the limit $R \to \infty$. Hence, the order of limiting processes is unimportant except in the vicinity of $k^2 = k_1^2$ and $k^2 = k_2^2$ or when $|\mathbf{k}_1| = |\mathbf{k}_2|$. (The last case requires special treatment and will not be considered here; in the following sections it is assumed that $|\mathbf{k}_1| \neq |\mathbf{k}_2|$.) The branch points in the pure Coulomb T matrix are due to that part of the potential beyond the screening radius R; Sec. V treats the effects of this part of the potential on the plane wave part of the pure Coulomb wave function.

II. SCREENED COULOMB T MATRIX

We begin by making an expansion in Legendre polynomials of the T matrix for an arbitrary central potential $V(r)$:

$$\langle \underset{\sim}{k}_2 | T | \underset{\sim}{k}_1 \rangle = \frac{\hbar^2}{4\pi^2 m} \sum_{\ell=0}^{\infty} (2\ell+1) P_\ell(\hat{k}_1 \cdot \hat{k}_2) \langle k_2 | T_\ell | k_1 \rangle . \tag{3}$$

The coefficients $\langle k_2 | T_l | k_1 \rangle$ are given by[3]

$$\langle k_2 | T_\ell | k_1 \rangle = \frac{2\pi^2 m}{\hbar^2} \int_{-1}^{1} \langle \underset{\sim}{k}_2 | T | \underset{\sim}{k}_1 \rangle P_\ell(\mu)\, d\mu \qquad (\mu = \hat{k}_1 \cdot \hat{k}_2) \tag{4}$$

and may be obtained by using Eq. (1) if the Green's function is known. This is accomplished by making an expansion of the coordinate representation of the Green's function:

$$\langle \underset{\sim}{r} | G | \underset{\sim}{r}' \rangle = \frac{2m}{\hbar^2} \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} P_\ell(\hat{r} \cdot \hat{r}') \langle r | G_\ell | r' \rangle . \tag{5}$$

After the angular integrations are carried out, we have

$$\langle k_2 | T_\ell | k_1 \rangle = B_\ell + M_\ell , \tag{6}$$

where

$$B_\ell = \int_0^\infty j_\ell(k_2 r)\, W(r)\, j_\ell(k_1 r)\, r^2\, dr \tag{7}$$

and

$$M_\ell = \int_0^\infty r^2\, dr \int_0^\infty r'^2\, dr'\, j_\ell(k_2 r)\, W(r) \langle r | G_\ell | r' \rangle W(r')\, j_\ell(k_1 r') \tag{8}$$

with $W(r) = (2m/\hbar^2)V(r)$.

To obtain the partial wave Green's function $\langle r | G_l | r' \rangle$, we write the operator equation $(E + i\epsilon - K - V)G = 1$ in the coordinate representation, which leads to

$$\left[\frac{1}{r}\frac{d^2}{dr^2}r + k^2 - \frac{\ell(\ell+1)}{r^2} - W(r)\right]\langle r|G_\ell|r'\rangle = \frac{\delta(r-r')}{r^2}. \tag{9}$$

The solution to this equation is easily shown to be

$$\langle r|G_\ell|r'\rangle = \frac{1}{ikrr'} F_\ell(r_<)\, H_\ell(r_>), \tag{10}$$

where $r_<$ is the smaller and $r_>$ the larger of r,r', and where F_l and H_l are the regular and irregular solutions of

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} - W(r)\right] f_\ell(r) = 0 \tag{11}$$

having the asymptotic forms

$$\begin{aligned} F_\ell(r) &\sim \cos\left[kr - \tfrac{1}{2}\pi(\ell+1) + \delta_\ell\right], \\ H_\ell(r) &\sim e^{i\left[kr - \frac{1}{2}\pi(\ell+1) + \delta_\ell\right]} \end{aligned} \tag{12}$$

With this normalization the Wronskian of F_l and H_l is equal to ik.

We now apply these formulas to the cutoff Coulomb potential

$$V(r) = \begin{cases} V_0/r & r < R \\ 0 & r > R \end{cases} \tag{13}$$

The solutions of Eq. (11) must in this case be proportional to pure Coulomb functions for $r < R$, and to free-particle functions for $r > R$. The Coulomb functions are normalized so that their Wronskian is equal to ik, and the free-particle functions are so chosen that the asymptotic forms of Eq. (12) are obtained for large r:

$$F_\ell(r) = \begin{cases} N_\ell F_\ell^c(r) & r < R \\ \frac{1}{2} kr \left[e^{i\delta_\ell} h_\ell^{(1)}(kr) + e^{-i\delta_\ell} h_\ell^{(2)}(kr) \right] & r > R \end{cases} \tag{14}$$

$$H_\ell(r) = \begin{cases} N_\ell^{-1} H_\ell^c(kr) & r < R \\ kr\, e^{i\delta_\ell} h_\ell^{(1)}(kr) & r > R . \end{cases} \tag{15}$$

Here $h_l^{(1)}$ and $h_l^{(2)}$ are spherical Hankel functions; the pure Coulomb functions F_l^c and H_l^c may be written[4]

$$F_\ell^c(r) = \frac{1}{2} C_\ell(\eta)(2kr)^{\ell+1} e^{ikr}\, \Phi(\ell+1+i\eta, 2\ell+2; -2ikr), \tag{16}$$

$$H_\ell^c(r) = e^{\frac{1}{2}\pi\eta + i\sigma_\ell} (-2kr)^{\ell+1} e^{ikr}\, \Phi(\ell+1+i\eta, 2\ell+2; -2ikr), \tag{17}$$

where

$$C_\ell(\eta) = e^{-\frac{1}{2}\pi\eta - i\sigma_\ell} \frac{\Gamma(\ell+1+i\eta)}{\Gamma(2\ell+2)} , \tag{18}$$

$$e^{2i\sigma_\ell} = \frac{\Gamma(\ell+1+i\eta)}{\Gamma(\ell+1-i\eta)} . \tag{19}$$

and $\eta = mV_0/\hbar^2 k$. The quantities N_l and δ_l are determined by equating logarithmic derivatives of F_l at $r = R$, but to first order in $1/R$ this is equivalent to matching amplitudes and phases; accordingly,

$$N_\ell \sim 1, \qquad \delta_\ell(k) \sim \sigma_\ell - \eta \ln(2kR). \tag{20}$$

For brevity we introduce the functions

$$u_\ell(r, K) \equiv r\, j_\ell(Kr)\, W(r)\, F_\ell^c(r) , \tag{21}$$

$$v_\ell(r, K) \equiv r\, j_\ell(Kr)\, W(r)\, H_\ell^c(r), \tag{22}$$

so that M_l may be written

$$M_\ell = \frac{1}{ik}\int_0^R u_\ell(r, k_2)\int_r^R v_\ell(r', k_1)\, dr'\, dr + \frac{1}{ik}\int_0^R v_\ell(r, k_2)\int_0^r u_\ell(r', k_1)\, dr'\, dr. \tag{23}$$

Now, by reversing the order of integration in the second term, we can show that

$$M_\ell = m_\ell(k_2, k_1) + m_\ell(k_1, k_2) = m_\ell + \tilde{m}_\ell , \tag{24}$$

where

$$m_\ell(k_2, k_1) = \frac{1}{ik}\int_0^R u_\ell(r, k_2)\int_r^R v_\ell(r', k_1)\, dr'\, dr. \tag{25}$$

In principle, therefore, evaluation of the cutoff Coulomb T matrix has been reduced to evaluation of $m_l(k_2,k_1)$ and the integral

$$B_\ell = 2\eta k\int_0^\infty j_\ell(k_2 r)\, j_\ell(k_1 r)\, r\, dr. \tag{26}$$

(A detailed study of the $l = 0$ terms $m_0(k_2,k_1)$ and B_0 is given in NASA TN D-2781.)

III. T MATRIX FOR LARGE R

The difficulty with the foregoing analysis is that it leads to expressions so complicated that the summation over l cannot be carried out in closed form.

Since in practice the screening radius is always very large, one is tempted to take the limit $R \to \infty$ in the hope that the resulting series can be summed. This approach is successful, but care must be taken when $k^2 \to k_1^2$ or $k^2 \to k_2^2$ because the limiting process is nonuniform.

We begin by rewriting m_l in the form

$$ik\, m_\ell = \int_0^\infty u_\ell(r) \int_r^\infty v_\ell(r')\, dr'\, dr - \left(\int_0^R u_\ell(r)\, dr\right)\left(\int_R^\infty v_\ell(r)\, dr\right) - \int_R^\infty u_\ell(r) \int_r^\infty v_\ell(r')\, dr'\, dr, \tag{27}$$

which is possible if u_l and v_l are given some suitable definition for $r > R$. For the present purpose it is convenient to require that u_l and v_l have the <u>same functional form</u> for $r > R$ as for $r < R$; i.e., u_l and v_l are proportional to pure Coulomb functions times spherical Bessel functions for <u>all</u> r. With this definition, the first term in Eq. (27) is just what one would write for the pure Coulomb[5] T matrix, and to emphasize this we write

$$m_\ell(R) = m_\ell(\infty) - \frac{1}{ik} U_\ell(R)\, V_\ell(R) + \mathcal{O}\left(\frac{1}{R}\right), \tag{28}$$

where

$$U_\ell(R) = \int_0^R u_\ell(r)\, dr \tag{29}$$

and

$$V_\ell(R) = \int_R^\infty v_\ell(r)\,dr. \qquad (30)$$

The third term in Eq. (27) has been dropped because, as shown in Appendix A, it is $\mathcal{O}(1/R)$ for all cases considered here.[6]

Generally speaking, the second term in Eq. (27) may also be neglected. To see this, consider the asymptotic forms of u_l and v_l,

$$u_\ell(r) \sim 2\eta k \frac{\sin(k_2 r - \frac{1}{2}\pi\ell)}{k_2 r} \sin\left[kr - \tfrac{1}{2}\pi\ell + \sigma_\ell - \eta \ln(2kr)\right], \qquad (31)$$

$$v_\ell(r) \sim -2i\eta k \frac{\sin(k_1 r - \frac{1}{2}\pi\ell)}{k_1 r} \frac{e^{i(kr - \frac{1}{2}\pi\ell + \sigma_\ell)}}{(2kr)^{i\eta}}. \qquad (32)$$

From Eq. (32) it follows, on integration by parts, that

$$V_\ell(R) = \frac{e^{ikR}}{(2kR)^{i\eta}}\, \mathcal{O}\left[\frac{1}{(k^2 - k_1^2)R}\right]. \qquad (33)$$

From Eq. (31) one can show that

$$\frac{e^{ikR}}{(2kR)^{i\eta}} \left[r\, u_\ell(r)\right]$$

is a bounded function of r for $r \le R$, $R \to \infty$; consequently, the quantity $e^{ikR}U_l(R)/(2kR)^{i\eta}$ has no worse than a logarithmic singularity as $R \to \infty$, and therefore

$$U_\ell(R)\, V_\ell(R) = \mathcal{O}\left[\frac{1}{(k^2 - k_1^2)R}\right]. \tag{34}$$

Equation (28) shows that $m_l(R)$ is given by its unscreened value $m_l(\infty)$ except when contributions to the latter from large r are important, and these occur only when $k^2 \to k_1^2$. Similar conclusions may be drawn for $\tilde{m}_l(R)$, the critical condition becoming $k^2 \to k_2^2$. Since $B_l(R) = B_l(\infty) + \mathcal{O}(1/R)$, we may write

$$\begin{aligned} \langle k_2 | T_\ell(k, R) | k_1 \rangle &= \langle k_2 | T_\ell(k, \infty) | k_1 \rangle + \mathcal{O}\left(\frac{1}{R}\right) \\ &\quad + \mathcal{O}\left[\frac{1}{(k^2 - k_1^2)R}\right] + \mathcal{O}\left[\frac{1}{(k^2 - k_2^2)R}\right], \end{aligned} \tag{35}$$

or, after the summation over l has been performed,

$$\begin{aligned} \langle \underset{\sim}{k}_2 | T(k, R) | \underset{\sim}{k}_1 \rangle &= \langle k_2 | T(k, \infty) | k_1 \rangle + \mathcal{O}\left(\frac{1}{R}\right) \\ &\quad + \mathcal{O}\left[\frac{1}{(k^2 - k_1^2)R}\right] + \mathcal{O}\left[\frac{1}{(k^2 - k_2^2)R}\right]. \end{aligned} \tag{36}$$

Now let us attempt to obtain a result more general than Eq. (36). This requires that we extract from the neglected terms and retain those parts which are important when $(k^2 - k_1^2)R \to 0$ or $(k^2 - k_2^2)R \to 0$. For this purpose the quantity $U_l V_l$ must be examined in greater detail.

We shall begin with V_l, which is given asymptotically by

$$V_\ell(R) \sim \frac{\eta k}{k_1}\, e^{i\sigma_\ell} \int_R^\infty \frac{e^{ikr}}{(2kr)^{i\eta}} \left[e^{-ik_1 r} + (-1)^{\ell+1} e^{ik_1 r} \right] \frac{dr}{r}. \tag{37}$$

A change to $t = r/R$ as the variable of integration yields

$$V_\ell(R) \sim \frac{k}{ik_1} e^{i\delta_\ell(k)} \left\{ f[(k-k_1)R] + (-1)^{\ell+1} f[(k+k_1)R] \right\}, \tag{38}$$

where

$$\begin{aligned} f(x) &\equiv i\eta \int_1^\infty t^{-1-i\eta} e^{ixt} dt \\ &= i\eta\, e^{ix}\, \Psi(1, 1-i\eta; -ix), \qquad |\arg(-ix)| < \tfrac{1}{2}\pi. \end{aligned} \tag{39}$$

The asymptotic form of $f(x)$ is easily found to be $-\eta e^{ix}/x$, while for values of x approaching zero, the relation

$$i\eta\, e^{ix}\, \Psi(1,1-i\eta;-ix) = \Phi(-i\eta, 1-i\eta; ix) - (-ix)^{i\eta}\Gamma(1-i\eta) \tag{40}$$

yields

$$f(x) \xrightarrow[x\to 0]{} 1 - (-ix)^{i\eta}\Gamma(1-i\eta). \tag{41}$$

When applied to $f\Big[(k - k_1) R\Big]$, Eq. (41) gives

$$\begin{aligned} f[(k-k_1)R] &= 1 - C_0(\eta)\, e^{-i\sigma_0} [(k_1-k)R]^{i\eta} + \mathcal{O}[(k-k_1)R] \\ &= 1 - C_0(\eta)\, e^{-i\delta_0(k)} \left(\frac{k_1^2 - k^2}{4k_1^2}\right)^{i\eta} + \mathcal{O}\Big[(k-k_1)R\Big], \end{aligned} \tag{42}$$

where

$$-2\pi < \arg(k_1^2 - k^2) < 0. \tag{43}$$

The corresponding result for $f\left[(k + k_1)R\right]$ is exactly the same, except that the neglected terms are, of course, $\mathcal{O}\left[(k + k_1)R\right]$. Combining these results, we have for the behavior of $f\left[(k \pm k_1)R\right]$ as $R \to \infty$

$$f\left[(k \pm k_1)R\right] = \begin{cases} \dfrac{e^{ikR}}{(2kR)^{i\eta}} \; \mathcal{O}\left[\dfrac{1}{(k^2 - k_1^2)R}\right] & \text{(44a)} \\[2ex] 1 - C_0(\eta)\, e^{-i\delta_0(k)} \left(\dfrac{k^2 - k_1^2}{4k_1^2}\right)^{i\eta} + \mathcal{O}\left[(k^2 - k_1^2)R\right]. & \text{(44b)} \end{cases}$$

Before proceeding, let us note that to $\mathcal{O}(1/R)$ the product $U_l V_l$ can be written in the form

$$A f\left[(k - k_1)R\right] + B f\left[(k + k_1)R\right] + \mathcal{O}\left(\frac{1}{R}\right),$$

where A and B are yet to be determined. We shall, in fact, be able to give exact expressions for A and B, valid for all k. However, since $f\left[(k - k_1)R\right]$ is already $\mathcal{O}(1/R)$ except when $k \to k_1$, an exact expression for A is really necessary only in the vicinity of $k = k_1$. Similarly, an exact expression for B is really necessary only in the vicinity of $k = -k_1$. For this reason we shall immediately put $k/k_1 = \pm 1$ in Eq. (38) and write

$$V_l(R) = -i e^{i\delta_l} \left\{ f\left[(k - k_1)R\right] + (-1)^l f\left[(k + k_1)R\right] \right\} + \mathcal{O}\left(\frac{1}{R}\right). \qquad (45)$$

Next we demonstrate that

$$\langle k_2 | T_l(k, R) | k \rangle = \frac{N_l\, e^{i\delta_l}}{k}\, U_l(R), \qquad (46)$$

i.e., U_l is proportional to $\langle k_2|T_l(k,R)|k_1\rangle$ for the special case where k_1 is complex and equal to k. The proof begins with the observation that Eqs. (6) to (8) may also be written as follows:

$$\langle k_2|T_l(k,R)|k\rangle = \int_0^\infty j_l(k_2 r)\, W(r)\, \psi_l(r)\, r^2\, dr, \tag{47}$$

where

$$\psi_l(r) = j_l(kr) + \int_0^\infty \langle r|G_l(k)|r'\rangle\, W(r')\, j_l(kr')\, r'^2\, dr' \tag{48}$$

and k_1 has been set equal to k.

Equation (48) is almost identical to one of the well-known integral equations for the radial wave function $F_l(r)$; it differs in that the wave numbers in $j_l(kr)$ and $G_l(k)$ are exactly equal instead of equal in the limit $\epsilon \to 0$. This circumstance makes the integrand in Eq. (48) a perfect derivative, however, and, as shown in Appendix B, the result is what one might naively expect:

$$\psi_l(r) = e^{i\delta_l}\, \frac{F_l(r)}{kr}\, . \tag{49}$$

Equations (47) and (49) then lead directly to the desired expression for $U_l(R)$.

As mentioned above, in order to determine $U_l V_l$ to $\mathcal{O}(1/R)$, the coefficient of $f\left[(k - k_1)R\right]$ must be known exactly only when $k = k_1$; therefore,

$$\frac{e^{i\delta_\ell}}{k} U_\ell(R) f[(k-k_1)R] = f[(k-k_1)R]\left[\frac{e^{i\delta_\ell}}{k} U_\ell(R)\right]_{k=k_1} + \mathcal{O}\left(\frac{1}{R}\right)$$

$$= f[(k-k_1)R] \langle k_2 | T_\ell(k_1, R) | k_1 \rangle + \mathcal{O}\left(\frac{1}{R}\right) \tag{50}$$

In like manner we may write

$$\frac{e^{i\delta_\ell}}{k} U_\ell(R) f[(k+k_1)R] = f[(k+k_1)R] \langle k_2 | T_\ell(-k_1, R) | -k_1 \rangle + \mathcal{O}\left(\frac{1}{R}\right)$$

$$= (-1)^\ell f[(k+k_1)R] \langle k_2 | T_\ell(-k_1, R) | k_1 \rangle + \mathcal{O}\left(\frac{1}{R}\right). \tag{51}$$

(The fact that $j_l(-x) = (-1)^l j_l(x)$ is used to obtain the final form of Eq. (51.) From Eqs. (45), (50), and (51) it follows that

$$m_\ell(R) = m_\ell(\infty) + f[(k-k_1)R] \langle k_2 | T_\ell(k_1, R) | k_1 \rangle$$

$$+ f[(k+k_1)R] \langle k_2 | T_\ell(-k_1, R) | k_1 \rangle + \mathcal{O}\left(\frac{1}{R}\right). \tag{52}$$

The expression for $\tilde{m}_l(R)$ is similar, but with k_1 and k_2 interchanged. Using the symmetry property

$$\langle k_1 | T_\ell(k) | k_2 \rangle = \langle k_2 | T_\ell(k) | k_1 \rangle \tag{53}$$

and its consequence

$$\langle \underset{\sim}{k}_1 | T(k) | \underset{\sim}{k}_2 \rangle = \langle \underset{\sim}{k}_2 | T(k) | \underset{\sim}{k}_1 \rangle \tag{54}$$

which can be readily established from Eqs. (7) and (8), we may give a general expression for the screened Coulomb T matrix, correct to $\mathcal{O}(1/R)$ and valid for all k:

$$\begin{aligned} \langle \underset{\sim}{k}_2 | T(k,R) | \underset{\sim}{k}_1 \rangle &= \langle \underset{\sim}{k}_2 | T(k,\infty) | \underset{\sim}{k}_1 \rangle \\ &+ f[(k-k_1)R] \langle \underset{\sim}{k}_2 | T(k_1,R) | \underset{\sim}{k}_1 \rangle \\ &+ f[(k+k_1)R] \langle \underset{\sim}{k}_2 | T(-k_1,R) | \underset{\sim}{k}_1 \rangle \\ &+ f[(k-k_2)R] \langle \underset{\sim}{k}_2 | T(k_2,R) | \underset{\sim}{k}_1 \rangle \\ &+ f[(k+k_2)R] \langle \underset{\sim}{k}_2 | T(-k_2,R) | \underset{\sim}{k}_1 \rangle + \mathcal{O}\left(\frac{1}{R}\right) \end{aligned} \tag{55}$$

IV. LIMITING CASES

To complete the study of the screened Coulomb T matrix, we shall need closed-form expressions for the T matrices that appear on the right side of Eq. (55). The first is the pure Coulomb T matrix with complex k, which may be obtained from Hostler's work and written as follows:

$$\langle \underset{\sim}{k}_2 | T(k,\infty) | \underset{\sim}{k}_1 \rangle = \frac{V_0}{2\pi^2} \frac{1 + I(x)}{(\underset{\sim}{k}_2 - \underset{\sim}{k}_1)^2} \tag{56}$$

where

$$I(x) = 2i\eta\left(1 - e^{-2\pi\eta}\right)^{-1} \int_{\infty}^{(1+)} \left(\frac{s-1}{s+1}\right)^{i\eta} \frac{1}{s^2 - x^2}\, ds\,, \tag{57}$$

$$x^2 = 1 + \frac{(k_2^2 - k^2)(k_1^2 - k^2)}{k^2(\underset{\sim}{k}_2 - \underset{\sim}{k}_1)^2}\,. \tag{58}$$

The integral $I(x)$ may be evaluated by changing to

$$t = \frac{s-1}{s+1}$$

as the variable of integration, with the result

$$I(x) = \frac{1}{x}\left[{}_2F_1\left(1, i\eta; 1+i\eta; \frac{x+1}{x-1}\right) - {}_2F_1\left(1, i\eta; 1+i\eta; \frac{x-1}{x+1}\right)\right]. \tag{59}$$

Considered as a function of k, $I(x)$ has simple poles at $i\eta = -n(n = 1,2,3\ldots)$ and branch points at $x^2 = 1$ and $x^2 = \infty$. These latter points correspond to $k^2 = k_1^2$, $k^2 = k_2^2$, $k^2 = 0$, and $k^2 = \infty$. The behavior of $I(x)$ as $x \to 1$ may be determined by analytic continuation of the hypergeometric series and is given by

$$I(x) \to C_0^2(\eta)\left(\frac{x-1}{x+1}\right)^{i\eta} - 1\,, \qquad -2\pi < \arg\left(\frac{x-1}{x+1}\right) < 0\,. \tag{60}$$

Applying this specifically to the case $k^2 \to k_1^2$, we can write

$$\langle \underset{\sim}{k}_2 | T(k,\infty) | \underset{\sim}{k}_1 \rangle \to \frac{V_0}{2\pi^2}\, C_0^2(\eta)\, \frac{(k_2^2-k^2)^{i\eta}}{[(\underset{\sim}{k}_2-\underset{\sim}{k}_1)^2]^{1+i\eta}} \left(\frac{k_1^2-k^2}{4k_1^2}\right)^{i\eta}, \tag{61}$$

where

$$-\pi < \arg(k_2^2-k^2) < \pi, \tag{62a}$$

$$-2\pi < \arg(k_1^2-k^2) < 0. \tag{62b}$$

Next we consider the screened Coulomb T matrices appearing in Eq. (55). All these can be obtained in closed form from the basic result of Ref. 2,

$$\langle \underset{\sim}{k}_2 | T(k,R) | \underset{\sim}{k}_1 \rangle \Big|_{k^2=k_1^2} = \frac{V_0}{2\pi^2}\, C_0(\eta)\, e^{i\delta_0(k)} \frac{(k_2^2-k^2)^{i\eta}}{[(\underset{\sim}{k}_2-\underset{\sim}{k}_1)^2]^{1+i\eta}} + \mathcal{O}\left(\frac{1}{R}\right). \tag{63}$$

Although Eq. (63) was originally derived with the assumption that $k = k_1$, it also holds for $k = -k_1$. To show this, we note from Eq. (1) that $T(E - i\epsilon) = T(E + i\epsilon)^*$, if V and K are real. From this, in the limit $\epsilon \to 0$,

$$T(k \to k_1 e^{\pi i}) = [T(k \to k_1)]^*.$$

Eq. (63) satisfies this relation and therefore holds for $k^2 = k_1^2$. The symmetry property (54) may be used to obtain the result for $k^2 = k_2^2$.

We can now see explicitly how the screened Coulomb T matrix behaves as $R \to \infty$. If k is complex, or is real but not equal to $\pm k_1$ or $\pm k_2$, all the f functions in Eq. (55) are $\mathcal{O}(1/R)$, and therefore

$$\lim_{R\to\infty} \langle \underset{\sim}{k}_2 | T(k,R) | \underset{\sim}{k}_1 \rangle = \langle \underset{\sim}{k}_2 | T(k,\infty) | \underset{\sim}{k}_1 \rangle$$
$$= \frac{V_0}{2\pi^2} \frac{1 + I(\chi)}{(\underset{\sim}{k}_2 - \underset{\sim}{k}_1)^2} \tag{64}$$

But when k approaches one of the critical values, say k_1, Eq. (55) reduces to

$$\langle \underset{\sim}{k}_2 | T(k,R) | \underset{\sim}{k}_1 \rangle = \langle \underset{\sim}{k}_2 | T(k,\infty) | \underset{\sim}{k}_1 \rangle$$
$$+ f[(k-k_1)R] \langle \underset{\sim}{k}_2 | T(k_1, R) | \underset{\sim}{k}_1 \rangle + \mathcal{O}\left(\frac{1}{R}\right). \tag{65}$$

The T matrix is thus represented by a combination of two terms, one correct for $R = \infty$, $k \neq k_1$, and the other correct for $k = k_1$, $R < \infty$; which term dominates is determined by $f\left[(k - k_1)R\right]$. If $R \to \infty$ faster than $k \to k_1$, the first term dominates, and we are led again to Eq. (64). As discussed previously, however, the limit $R \to \infty$ is actually a convenience and should be performed last, which corresponds to $(k - k_1)R \to 0$. Comparing Eq. (44b) to the T matrices as given in Eqs. (61) and (63) reveals that in this situation a cancellation takes place and yields

$$\langle \underset{\sim}{k}_2 | T(k,R) | \underset{\sim}{k}_1 \rangle = \langle \underset{\sim}{k}_2 | T(k_1, R) | \underset{\sim}{k}_1 \rangle + \mathcal{O}\left[(k-k_1)R\right] + \mathcal{O}\left(\frac{1}{R}\right)$$
$$= \frac{V_0}{2\pi^2} C_0(\eta)\, e^{i\delta_0} \frac{(k_2^2 - k^2)^{i\eta}}{[(\underset{\sim}{k}_2 - \underset{\sim}{k}_1)^2]^{1+i\eta}} + \mathcal{O}\left[(k-k_1)R\right] + \mathcal{O}\left(\frac{1}{R}\right). \tag{66a}$$

In the general case, where $(k - k_1)R$ approaches some fixed value as $R \to \infty$, use of Eq. (40) leads to

$$\langle \underset{\sim}{k}_2 | T(k,R) | \underset{\sim}{k}_1 \rangle = \langle \underset{\sim}{k}_2 | T(k_1,R) | \underset{\sim}{k}_1 \rangle \, \Phi[-i\eta, 1-i\eta; i(k-k_1)R] + \mathcal{O}\left(\frac{1}{R}\right). \qquad (66b)$$

Obviously, similar results are obtained when k approaches any of the other critical values.

We may summarize our findings as follows: Generally, it makes no difference when the limit $R \to \infty$ is taken in the expression for the screened Coulomb T matrix; the result is identical to the pure Coulomb T matrix and does not depend on R. The exception to this generalization occurs when k^2 approaches k_1^2 or k_2^2. In this case the screened Coulomb T matrix admits of an asymptotic expansion, the leading term of which is a well-behaved function of k and depends on R through the logarithmic phase factor $e^{i\delta_o}$. In contrast, the pure Coulomb T matrix has branch points at k_1^2 and k_2^2, in addition to being independent of R.

Near these critical points, the difference between the pure and screened Coulomb T matrices is due to contributions to the latter from $r' > R$. These contributions do not affect the angular dependence of the T matrix, but only its magnitude and phase. The effect on the magnitude is such as to make the T matrix discontinuous in the limit $R \to \infty$. This effect is strikingly displayed when k is on the real axis; near k_1, for instance, we have

$$\lim_{R \to \infty} \left| \langle \underset{\sim}{k}_2 | T(k,R) | \underset{\sim}{k}_1 \rangle \right| = \frac{V_0}{2\pi^2} \frac{1}{(\underset{\sim}{k}_2 - \underset{\sim}{k}_1)^2} \mathfrak{M}_1 \mathfrak{M}_2 \, , \qquad (67)$$

where

$$\mathcal{M}_1 = \begin{cases} C_0(\eta) & k_1 > k \\ 1 & k_1 = k \\ e^{\pi\eta} C_0(\eta) & k_1 < k \end{cases} ; \qquad \mathcal{M}_2 = \begin{cases} C_0(\eta) & k_2 > k_1 \\ e^{\pi\eta} C_0(\eta) & k_2 < k_1 . \end{cases} \tag{68}$$

V. WAVE FUNCTIONS

A remarkable finding of the preceding section is that when k^2 approaches k_1^2 or k_2^2, the entire contribution to the pure Coulomb T matrix comes from large values of r'. More precisely, the contribution from $r' > R$ consists of two parts identical except in normalization, one of which exactly cancels the contribution from $r' < R$. When screening is introduced, the cancellation is prevented. It is perhaps worth noting that this same phenomenon is responsible for the well-known distortion of the incident plane wave in a pure Coulomb field.

To see this, consider the wave operator $\Omega(k)$, which is related to the Green's function by the equation

$$\Omega(k) = 1 + G(k)V. \tag{69}$$

Suppose that $\Omega(k)$ operates on a plane wave of momentum $\hbar k_1$, with $k \neq |\underset{\sim}{k}_1|$. A partial wave expansion yields

$$\Omega(k)\,\phi_{\underset{\sim}{k}_1} = (2\pi)^{-\frac{3}{2}} \sum_{\ell=0}^{\infty} i^{\ell}(2\ell+1)\, P_\ell(\hat{r}\cdot\hat{k}_1)\; R_\ell(r), \tag{70}$$

where

$$R_\ell(r) = j_\ell(k_1 r) + \int_0^\infty \langle r | G_\ell(k) | r' \rangle W(r') j_\ell(k_1 r') r'^2 dr'. \tag{71}$$

(The radial function $R_l(r)$ is generally different from $\psi_l(r)$ of Sec. IV, because the wave numbers in $j_l(k_1 r)$ and $G_l(k)$ are different.) By making use of quantities defined in previous sections, we may develop the following exact expression for $R_l(r)$:

$$R_\ell(r) = j_\ell(k_1 r) + \frac{1}{ikr}\left\{ N_\ell H_\ell(r) U_\ell(r_<, k_1) + N_\ell^{-1} F_\ell(r)\left[V_\ell(r_<) - V_\ell(R)\right]\right\}, \tag{72}$$

where $r_<$ is the smaller of r and R. (We have written $U_l(r_<, k_1)$ to indicate explicitly that k_1 is involved, not k_2 as before.)

Now let us determine the asymptotic form of $R_l(r)$. Since $k^2 \neq k_1^2$, we have $V_l(r) = e^{ikr}\mathcal{O}(1/r)$ as before. Thus, if we suppose $r_<$ to be large enough that $N_l \sim 1$,

$$R_\ell(r) \sim j_\ell(k_1 r) + \frac{1}{ikr}\left[H_\ell(r) U_\ell(r_<, k_1) + \mathcal{O}\left(\frac{1}{r_<}\right)\right]$$

$$\sim j_\ell(k_1 r) - \frac{e^{ikr}}{r} (-i)^\ell \langle k | T_\ell(k, r_<) | k_1 \rangle + \mathcal{O}\left(\frac{1}{r_<^2}\right). \tag{73}$$

This equation may be inserted into Eq. (70) and the summation over l performed, which yields

$$\Omega(k)\,\phi_{\underset{\sim}{k}_1} \sim (2\pi)^{-\frac{3}{2}}\left[e^{i\underset{\sim}{k}_1\cdot\underset{\sim}{r}} - \frac{e^{ikr}}{r}\langle\underset{\sim}{k}|T_\ell(k,r_<)|\underset{\sim}{k}_1\rangle\right], \tag{74}$$

where $\underset{\sim}{k} \equiv k\underset{\sim}{r}/r$. The "scattering amplitude" $-\langle\underset{\sim}{k}|T(k,r_<)|\underset{\sim}{k}_1\rangle$ depends only weakly on $r_<$, through a logarithmic phase factor $e^{-i\eta\ln(2kr_<)}$; the plane wave $e^{i\underset{\sim}{k}_1\cdot\underset{\sim}{r}}$ is unaffected.

Although Eq. (74) has been derived assuming a cutoff Coulomb potential for $W(r)$, this restriction is not necessary. We can return to Eq. (72), set $R = \infty$, and proceed as before; now the only reference to a cutoff potential is to identify $U_l(r,k_1)$ as proportional to $\langle k|T_l(k,r)|k_1\rangle$. Thus we conclude that even in a pure Coulomb field, the incident plane wave is undistorted if $k^2 \neq k_1^2$.

However, if $k^2 \to k_1^2$, the result depends critically on when the limit $R \to \infty$ is taken. Equation (74) is still valid when $k^2 = k_1^2$ provided that $r \geq R$, i.e., the limit $R \to \infty$ is taken last. Here the factor $V_l(r_<) - V_l(R)$ in Eq. (72) prevents any cancellation due to contributions from $r' > R$. But if the limit $R \to \infty$ is taken first, the term $F_l(r)V_l(r)$ survives and becomes important as $k^2 \to k_1^2$. Now cancellation does take place, and after some rearrangement we find that

$$R_\ell(r) \sim C_0(\eta)\left(\frac{k_1^2 - k^2}{4k_1^2}\right)^{i\eta} e^{i\sigma_\ell}\,\frac{F_\ell^c(r)}{kr} + \mathcal{O}\left(\frac{1}{r_<^2}\right) \tag{75}$$

or

$$\Omega(k)\phi_{\underset{\sim}{k}_1} \sim C_0(\eta)\left(\frac{k_1^2-k^2}{4k_1^2}\right)^{i\eta}\psi^c_{\underset{\sim}{k}_1}(\underset{\sim}{r}) \tag{76}$$

where $\psi^c_{\underset{\sim}{k}_1}(\underset{\sim}{r})$ is the pure Coulomb wave function.[7] As is well known, $\psi^c_{\underset{\sim}{k}_1}$ is given asymptotically by a scattered wave plus a distorted plane wave. We also note from Eq. (76) that $\Omega(k)\varphi_{\underset{\sim}{k}_1}$ does not have unit amplitude for large r, a fact first pointed out by Mapleton.[8] Both these features which appear as $k^2 \to k_1^2$, the plane wave distortion and the amplitude renormalization, are due to (unphysical) contributions from $r' > R$.

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APPENDIX A - ORDER OF MAGNITUDE OF $\int_R^\infty u_l V_l \, dr$

In the text, the third term in Eq. (27), which may be written

$$\int_R^\infty u_l(r) V_l(r) \, dr, \tag{A1}$$

was neglected on the premise that it is always $\mathcal{O}(1/R)$ for cases of interest. To prove this, we first observe that (using the asymptotic form of u_l) the integral may be decomposed into four integrals of the type

$$\int_R^\infty \frac{e^{i\lambda r}}{r^{1+i\nu\eta}} V_l(r) \, dr, \tag{A2}$$

where λ and ν take on the values $\nu(k \pm k_2)$ and ± 1, respectively. From Eq. (33) for $V_l(r)$, we see immediately that $e^{i\lambda r} V_l(r)/r^{i\nu\eta} = \mathcal{O}(1/r)$ unless $k^2 \to k_1^2$; therefore

$$\int_R^\infty u_l V_l \, dr = \mathcal{O}\left[\frac{1}{(k^2 - k_1^2)R}\right]. \tag{A3}$$

To derive an expression valid when $k^2 \to k_1^2$, we integrate (A2) by parts and obtain

$$\frac{1}{i\lambda}\left\{ \frac{e^{i\lambda r}}{r^{1+i\nu\eta}} V_l(r) \Big|_{r=R}^{r=\infty} + \int_R^\infty \frac{e^{i\lambda r}}{r^{1+i\nu\eta}} \left[\frac{1+i\nu\eta}{r} V_l(r) + v_l(r)\right] dr \right\}, \tag{A4}$$

since $dV_l/dr = -v_l$. From Eqs. (38) - (41) we can show that, for all values of k, $e^{i\lambda r}V_l(r)/r^{i\nu\eta}$ is bounded and $e^{i\lambda r}v_l(r)/r^{i\nu\eta}$ is $\mathcal{O}(1/r)$ as $r \to \infty$. Consequently, (A4) is $\mathcal{O}(1/\lambda R)$, which leads to

$$\int_R^\infty u_l V_l \, dr = \mathcal{O}\left[\frac{1}{(k^2 - k_2^2)R}\right]. \tag{A5}$$

Eqs. (A3) and (A5) indicate that the integral is negligible unless $k_1^2 = k_2^2$, which is excluded from the present discussion.

APPENDIX B - EVALUATION OF $\psi_l(kr)$

In Eq. (48) we encounter the integral

$$P = \int_0^\infty \langle r | G_\ell(k) | r' \rangle \, W(r') \, j_\ell(kr') \, r'^2 \, dr',$$

which may be written explicitly as

$$P = \frac{1}{ik^2 r} \left[F_\ell(r) \int_r^\infty H_\ell(r') W(r') \mathcal{F}_\ell(r') \, dr' + H_\ell(r) \int_0^r F_\ell(r') W(r') \mathcal{F}_\ell(r') \, dr' \right],$$

where $\mathcal{F}_l(r) \equiv krj_l(kr)$. Recalling that $F_l(r)$ and $H_l(r)$ are both solutions of

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} - W(r)\right] f_\ell(r) = 0,$$

and observing that $\mathcal{F}_l(r)$ satisfies a similar equation but with $W(r) \equiv 0$, we can readily verify that

$$f_\ell(r) W(r) \mathcal{F}_\ell(r) = \frac{d}{dr}\left(\mathcal{F}_\ell \frac{df_\ell}{dr} - f_\ell \frac{d\mathcal{F}_\ell}{dr}\right) = \frac{d}{dr} W(\mathcal{F}_\ell, f_\ell),$$

where $W(\mathcal{F}_l, f_l)$ is the Wronskian of $\mathcal{F}_l$ and f_l. Therefore,

$$P = \frac{1}{ik^2 r} \left[F_\ell(r) \, W(\mathcal{F}_\ell, H_\ell) \Big|_{r'=r}^{r'=\infty} + H_\ell(r) \, W(\mathcal{F}_\ell, F_\ell) \Big|_{r'=0}^{r'=r} \right],$$

and after some rearrangement,

$$P = \frac{1}{ik^2 r}\Big[\, F_\ell(r)\, W(\mathcal{F}_\ell, H_\ell)_{r'=\infty} - \mathcal{F}_\ell(r)\, W(F_\ell, H_\ell)_{r'=r}$$

$$- H_\ell\, W(\mathcal{F}_\ell, F_\ell)_{r'=0}\Big].$$

Since both F_l and $\mathcal{F}_l$ vanish as $(kr)^{l+1}$ when $kr \to 0$, the last term is zero. The Wronskian of F_l and H_l is equal to ik, and From Eq. (12) one can establish that as $kr \to \infty$,

$$W(\mathcal{F}_\ell, H_\ell) \to ik\, e^{i\delta_\ell(k,r)}.$$

For the cutoff Coulomb potential, the upper limit for the integral P should actually be $r' = R$, and thus finally

$$P = e^{i\delta_\ell(k,R)}\, \frac{F_\ell(r)}{kr} - j_\ell(kr).$$

This equation leads immediately to the result given in Eq. (49).

FOOTNOTES

1. L. Hostler, J. Math. Phys. **5**, 591 (1964); J. Schwinger, idid. **5**, 1606 (1964); E. H. Wichmann and C. H. Woo, ibid. **2**, 178 (1961).
2. W. F. Ford, Phys. Rev. **133B**, 1616 (1964).
3. The expansion here differs by a minus sign from that used in Ref. 2.
4. Notation and formulas for the confluent hypergeometric functions Φ and Ψ are taken from Higher Transcendental Functions, Bateman Manuscript Project (McGraw-Hill Book Co., Inc., New York 1953), Vol. I, Chap. 6.
5. By "pure Coulomb" we shall mean a quantity obtained by assuming $R = \infty$ at the outset, as opposed to taking the limit $R \to \infty$ at the last.
6. For simplicity, the symbol $\mathcal{O}(1/x)$ is used loosely throughout to denote any term which vanishes when $x \to \infty$.
7. Eq. (76) is actually an identity holding for all r, not an asymptotic equality. This can be proved by using the integral representation (56) in the relation $\Omega = 1 + (E + i\epsilon - K)^{-1}T$ and taking the limit $k^2 \to k_1^2$. The result is proportional to an integral representation for the pure Coulomb wave function.
8. R. A. Mapleton, J. Math. Phys. **3**, 297 (1962).